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Lecture 07: Nonlinear Preconditioning Methods and Applications

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Nonlinear Preconditioning Methods and Applications

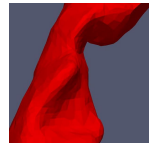
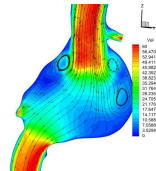
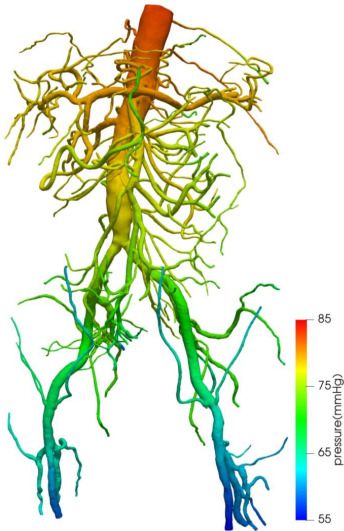
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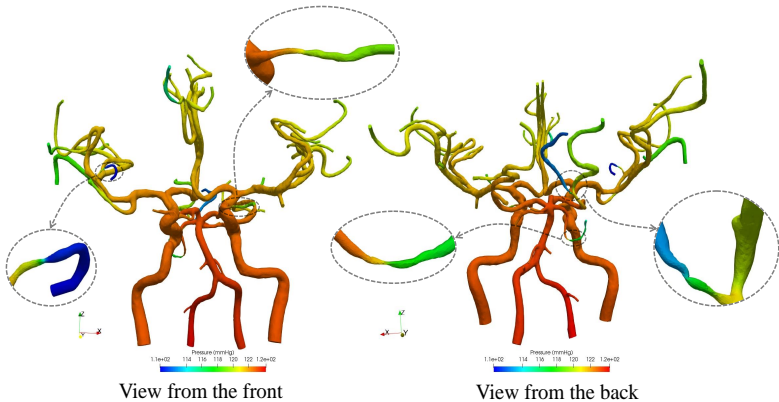
Outline of the talk

- Root Finding Problem: Find $X \in R^n$, such that $F(X) = 0$
- Motivating applications
- Nonlinearly preconditioned Newton methods
- Some nonlinearly difficult problems in fluid and solid problems in biomechanics
- Final remarks

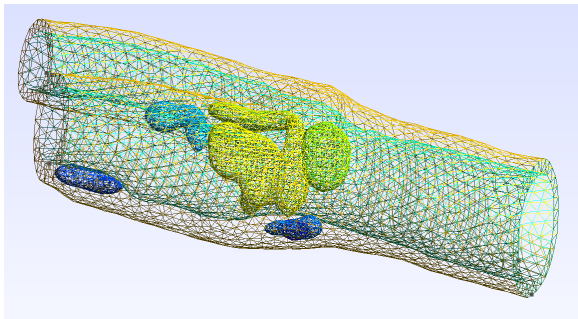
Nonlinear problems with
local singularity: Blood
flows in arteries with
aneurysm or stenosis



Nonlinear problems with local singularity: Stroke



Nonlinear problems with local singularity: Arterial plaques



Motivation from linear preconditioning

- Iterative methods for solving large system of linear equations

$$Ax = b$$

Roughly speaking, if h is the mesh size and np is the number of processors of a parallel machine

- The discretization accuracy $\approx h^\alpha$
- The number of iterations $\approx h^{-\beta} \cdot (np)^\gamma$
- Preconditioned iterative methods for solving large system of linear equations

$$M^{-1}Ax = M^{-1}b$$

- A good preconditioner reduces the impact of certain parameters on the convergence. Parameters: mesh size, number of processors, jump coefficients, ...

- Preconditioned iterative methods for solving large system of nonlinear equations

$$F(X) = 0 \iff G(F(X)) = 0 \iff F(G(X)) = 0$$

- A good nonlinear preconditioner can sometimes drastically improve the robustness of the nonlinear convergence by reducing the impact of certain parameters on the nonlinear convergence
- Parameters: Reynolds number, Mach number, Grashof number, ..., plus mesh size, number of processors, ...
- **Note:** Linear preconditioning doesn't help much with the “nonlinear parameters”

A little history of nonlinear preconditioning

- X.-C. Cai, W. D. Gropp, D. E. Keyes, R. G. Melvin, and D. P. Young, Parallel Newton-Krylov-Schwarz algorithms for the transonic full potential equation, SIAM J. Sci. Comput., 19 (1998), pp. 246-265.
(a shock wave problem)
- X.-C. Cai, D. E. Keyes, and D. P. Young, A nonlinear additive Schwarz preconditioned inexact Newton method for shocked duct flow, Proceedings of the 13th International Conference on Domain Decomposition Methods, Oct. 9-12, 2000, France.
(a shock wave problem solved using nonlinear preconditioning)
- X.-C. Cai and D. E. Keyes, Nonlinearly preconditioned inexact Newton algorithms, SIAM J. Sci. Comput., 24 (2002), pp. 183-200.
(left nonlinear preconditioning)
- X.-C. Cai and X. Li, Inexact Newton methods with restricted additive Schwarz based nonlinear elimination for problems with high local nonlinearity, SIAM J. Sci. Comput., 33 (2011), pp. 746-762.
(right nonlinear preconditioning)

In general, we can use **the classical Newton's method** for

$$F(X) = 0,$$

where $X = (x_1, x_2, \dots, x_n)^T$ and $F = (f_1, f_2, \dots, f_n)^T$

$$X^{k+1} = X^k - F'(X^k)^{-1} F(X^k)$$

or, equivalently,

$$X^{k+1} = X^k + H^k$$

$$F'(X^k)H^k = -F(X^k),$$

which requires the solving of a large linear system of equations at every iteration

Inexact Newton's method: H^k is chosen such that

$$\|F'(X^k)H^k + F(X^k)\| \leq \eta^k \|F(X^k)\|,$$

for a given $\eta^k > 0$ (which may or may not depend on k)

Globally convergent Newton's methods

- Linesearch: Changing the steplength by a factor of $\lambda^k \in (0, 1]$

$$X^{k+1} = X^k - \lambda^k H^k$$

In other words, H^k is a good search direction if a non-zero λ^k can be found such that

$$\frac{1}{2} \|F(X^{k+1})\|^2 \leq \frac{1}{2} \|F(X^k)\|^2 - \alpha \lambda^k (H^k)^T JF(X^k)$$

where α is small positive parameter

- Trust region: Changing the search direction H^k

What happens when inexact Newton is applied to a large system with unbalanced nonlinearities?

- The convergence, or fast convergence, happens only if a good initial guess is available
- Generally it is very difficult to obtain such an initial guess especially for nonlinear equations that have unbalanced nonlinearities
- The step length λ^k is often determined by the components with the strongest nonlinearities, and this may lead to an extended period of stagnation in the nonlinear residual curve
- We say that the nonlinearities are “unbalanced” when λ^k is, in effect, determined by a subset of the overall degrees of freedom

We consider a one-dimensional compressible flow problem described by the full potential equation in a variable-area duct. The problem is to determine the solution potential $u(x)$ satisfying

$$(A\rho u_x)_x = 0,$$

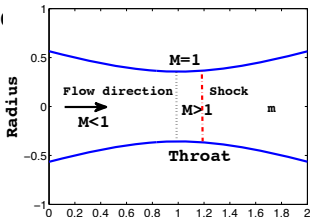
for $0 < x < 2$ and $u(0) = 0$ and $u(2) = u_R$ given. The duct area

$$A = A(x) = 0.4 + 0.6(x - 1)^2,$$

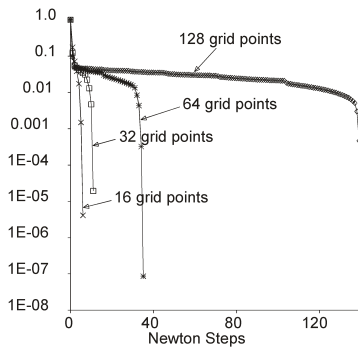
and the density ρ is given by

$$\rho = \rho(v) = (c^2)^{1/(\gamma-1)} = \left(1 + \frac{\gamma-1}{2}(1 - v^2)\right)^{1/(\gamma-1)}.$$

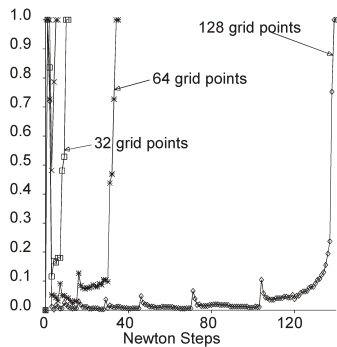
Here $v = u_x$ is the velocity. $\gamma = 1.4$ is the ratio of specific heat and c is the speed of sound.



Relative Residual



Step Length



Some observations

- To advance from X^k to X^{k+1} , all n variables and equations need to be updated even though in many situations n can be very large, but only a small number of components of X^k receive significant updates
- If a small number of components of the initial guess X^0 are not acceptable, the entire X^0 is declared bad
- There are two global control variables η^k and λ^k . Any slight change of $F(\cdot)$ may result in the change of η^k or λ^k , and any slight change of η^k or λ^k may result in some global function evaluations and/or the solving of global Jacobian systems

Can we remove those bad components, just like Gaussian elimination?

For example

$$\begin{cases} F_1(x_1, x_2) = 0 \\ F_2(x_1, x_2) = 0 \end{cases}$$

Eliminate (implicit function theorem) the bad component x_2

$$x_2 = G(x_1)$$

The leftover is a slightly smaller and easier to solve nonlinear system

$$F_1(x_1, G(x_1)) = 0$$

A simple example with one bad component

- Consider a 2×2 system

$$F(x_1, x_2) \equiv \begin{bmatrix} F_1(x_1, x_2) \\ F_2(x_1, x_2) \end{bmatrix} = \begin{bmatrix} (x_1 - x_2^3 + 1)^m - x_2^m \\ x_1 + 2x_2 - 3 \end{bmatrix} = 0$$

where $m = 1, 3, 5$. $x^* = [1, 1]^T$ is the root

	IN			PIN		
$x^{(0)}$	$m=1$	$m=3$	$m=5$	$m=1$	$m=3$	$m=5$
$(0, 0)^T$	5	8	10	5	6	6
$(0, 2)^T$	5	11	12	5	6	6
$(2, 0)^T$	5	1	7	5	1	5
$(2, 2)^T$	5	12	13	5	5	6

- As m increases, one of the equations is more nonlinear than the other; the number of iterations increases and is also more sensitive to the choice of the initial guess

Nonlinear elimination – peak removing

Consider a nonlinear problem $F(x) = 0$ defined on Ω with the current approximate solution x_c .

- Identify the worst region. A peak of F is a region $\omega \in \Omega$ such that $\|F(x_c)\|_{2(\omega)}$ is large
- Solve a local nonlinear problem

$$F|_{\omega}(x_{\omega}) = 0, \text{ with boundary condition } x_{\omega}|_{\partial\omega} = x_c|_{\partial\omega}$$

- Locally correct the solution

$$x_{new} = \begin{cases} x_{\omega} & \text{in } \omega \\ x_c & \text{in } \Omega \setminus \omega \end{cases}$$

Linear and nonlinear Schwarz preconditioners

- R_i^δ, R_i^0 restriction with and without overlap. δ is the overlapping size
- Additive Schwarz

$$\text{Linear: } \sum_{i=1}^N (R_i^\delta)^T A_i^{-1} R_i^\delta \quad \text{Nonlinear: } \sum_{i=1}^N (R_i^\delta)^T F_i^{-1}(R_i^\delta x)$$

- Restricted additive Schwarz

$$\text{Linear: } \sum_{i=1}^N (R_i^0)^T A_i^{-1} R_i^\delta \quad \text{Nonlinear: } \sum_{i=1}^N (R_i^0)^T F_i^{-1}(R_i^\delta x)$$

A general scalable nonlinear equation solver: RAS-NKS

- **Step 1 (The Nonlinearity Checking Step):** Check stopping conditions.
 - If the global condition is satisfied, **stop**.
 - If the local nonlinearities are not balanced, go to **Step 2**.
 - If the local conditions indicate the nonlinearities are balanced, set $\tilde{u}^{(k)} = u^{(k)}$, go to **Step 3**.
- **Step 2 (The RAS Step):** Solve local nonlinear problems on the overlapping subdomains to obtain the subdomain correction v_i^δ

$$R_i^\delta F(u^{(k)} + v_i^\delta) = 0, \text{ for } i = 1, \dots, N$$

Drop the solution in the overlapping part of the subdomain and compute the global function $G(u^{(k)})$

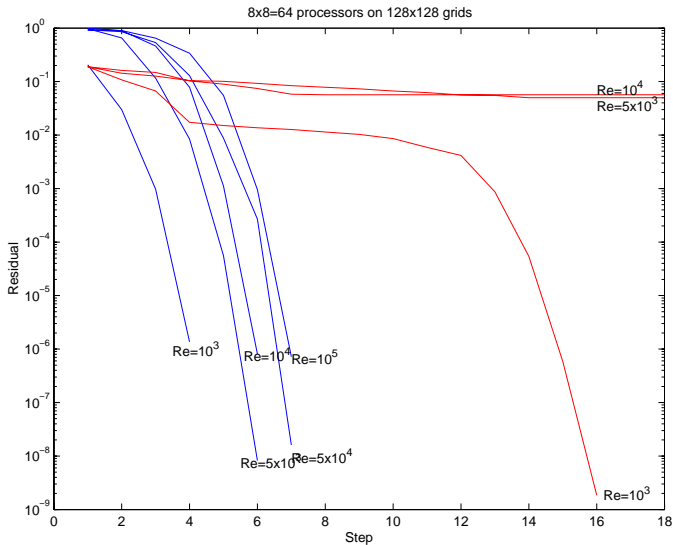
$$G(u^{(k)}) = \sum_{i=1}^N R_i^0(u^{(k)} + v_i^\delta), \text{ and set } \tilde{u}^{(k)} = G(u^{(k)}).$$

- **Step 3 (The NKS Step):** Compute the next approximate solution $u^{(k+1)}$ by solving the following equation

$$F(u) = 0$$

with one step of NKS iteration using $\tilde{u}^{(k)}$ as the initial guess.
Go to **Step 1**

Comparing NKS and RAS-NKS

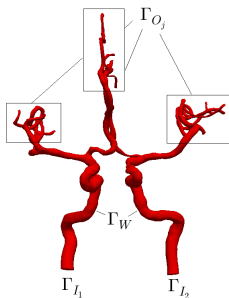


Blood flow in the cerebral artery of a stroke patient

Time-dependent incompressible Navier-Stokes equations

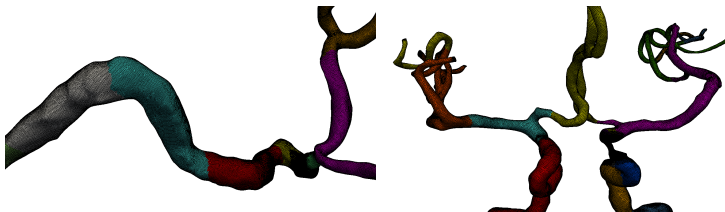
$$\begin{cases} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) - \nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

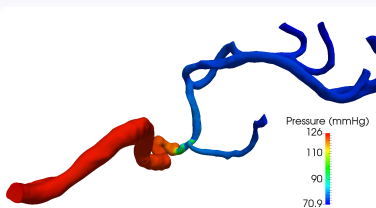
Here ρ is the blood density, μ is the viscosity, and $\boldsymbol{\sigma} = -p\mathbf{I} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the Cauchy stress tensor, \mathbf{u} is the velocity, p is the pressure.



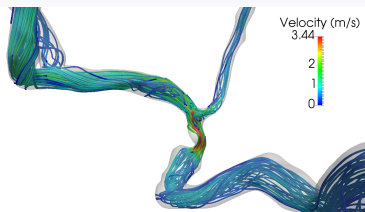
Two cases of patient-specific arteries

Case	Mean Reynolds	# of inlets	# of outlets	# of nodes	# of elements
One-inlet	443.2	1	6	437,538	2,190,164
Two-inlet	262.6	2	15	1,069,767	5,225,949

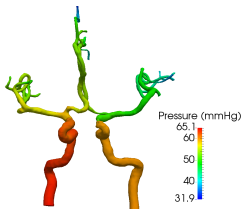




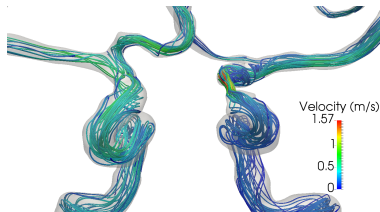
(a) Pressure



(b) Streamlines



(c) Pressure



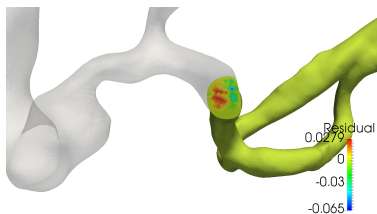
(d) Streamlines

Figure: Numerical solutions at $t = 0.7s$.

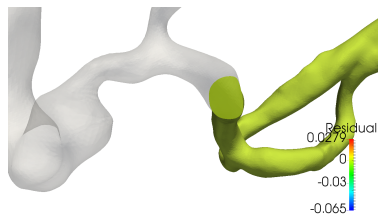
We form the following nonlinear system in the region with large residuals

$$\mathcal{G}(\mathbf{x}) \equiv \mathcal{R}_b^k(\mathcal{F}(\mathbf{x})) + \mathcal{R}_g^k(\mathbf{x} - \mathbf{x}_k^n) = \mathbf{0}.$$

\mathbf{x}_k^* is accepted as the approximate solution if the stopping condition $\|\mathcal{G}(\mathbf{x}_k^*)\| \leq \gamma_r^{NE} \|\mathcal{G}(\mathbf{x}_k^n)\|$ is satisfied.



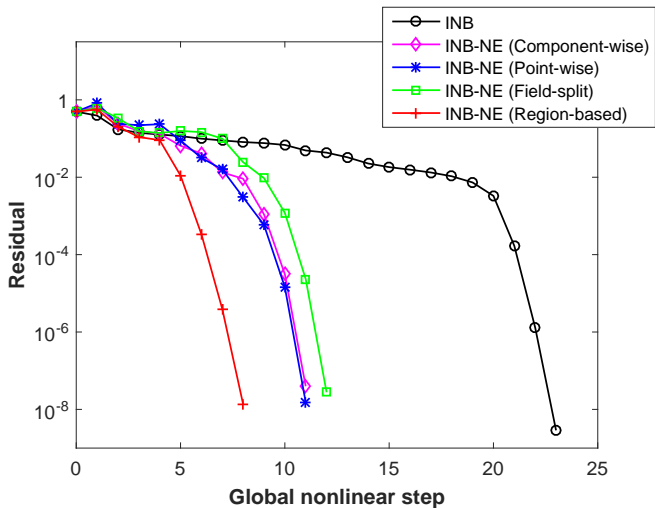
(a) Before the subspace correction



(b) After the subspace correction

Figure: The one-inlet case: residual contours for the u component at the second nonlinear step during the second time step.

Nonlinear residual history

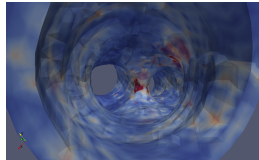
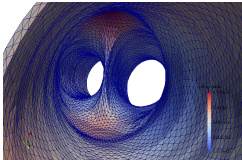
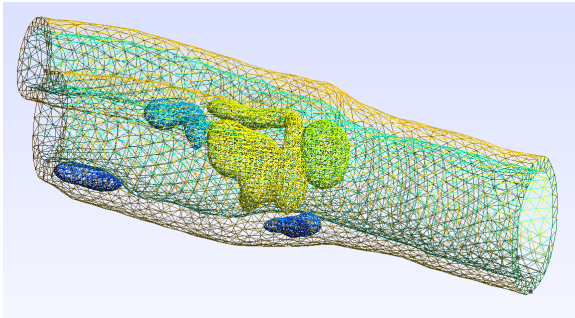


Parallel scalability of INB-NE

Table: Scalability test for the two-inlet case obtained using the INB-NE method with different fill-in levels of the ILU subsolve. A fixed mesh with 5,225,949 elements and 1,069,767 nodes is used. The overlap size of RAS preconditioner is $\delta = 1$. The time step size is 0.0025s.

np	Subsolve	NI_{global}	LI_{global}	NI_{ne}	LI_{ne}	$Time_{ne}(s)$	$Time_{total}(s)$
240	ILU(0)	3.83	1068.52	1.33	6.75	11.04	243.79
	ILU(1)	3.67	668.59	1.20	3.66	10.42	171.54
	ILU(2)	3.83	525.70	1.20	3.33	10.82	171.83
	ILU(3)	3.50	488.47	1.20	3.00	11.54	179.63
480	ILU(0)	3.83	1115.04	1.33	6.50	6.19	133.81
	ILU(1)	3.50	683.47	1.20	4.00	5.83	87.84
	ILU(2)	3.67	532.91	1.20	3.67	6.05	88.66
	ILU(3)	3.50	491.91	1.20	3.50	6.47	96.40
960	ILU(0)	3.83	1179.70	1.33	6.63	3.72	77.45
	ILU(1)	3.50	743.81	1.20	4.00	3.69	52.88
	ILU(2)	3.50	541.76	1.20	3.67	3.76	48.08
	ILU(3)	3.67	505.50	1.20	3.50	4.02	56.74
1920	ILU(0)	3.83	1436.56	1.20	5.00	2.27	53.17
	ILU(1)	3.67	900.36	1.20	4.16	2.30	38.33
	ILU(2)	3.67	653.05	1.20	3.67	2.34	33.31
	ILU(3)	3.67	630.18	1.20	3.83	2.43	38.58

A carotid artery with plaques



Hyperelastic model for arterial wall

- Energy functional

$$\psi = \psi^{iso}(C) + \psi^{vol}(C) + \psi^{ti}(C, M^{(i)}),$$

where C is Cauchy-Green tensor,
 $M^{(i)}$ are the structural tensors

- Momentum equation

$$\text{div} P = -f$$

where $P = FS$, $S = \frac{\partial \psi}{\partial C}$

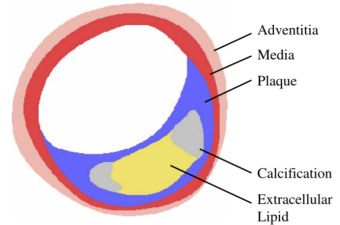


Figure: Cross-section of artery [Klawonn et al., 2008]

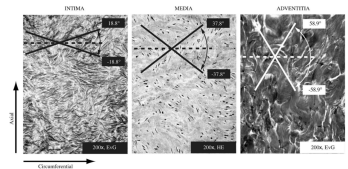


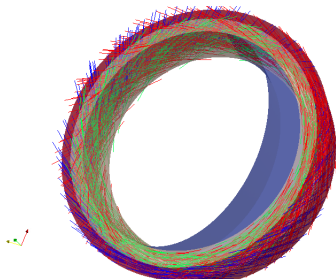
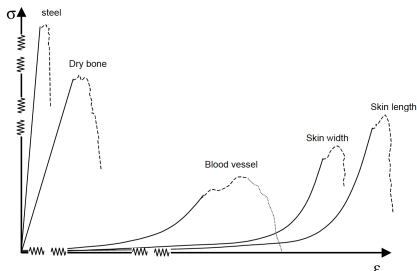
Figure: Collagen fibre reinforced [Holzapfel et al., 2000]

Computational difficulties

Standard NKS doesn't work well under the following 3 conditions, and **the issue is not the linear solver**

- Large deformation
- Nearly incompressible
- Highly anisotropic

Material	Poisson's Ratio
rubber	0.4999
soft tissue	0.45 - 0.49
gold	0.42 - 0.44
clay	0.3 - 0.45
stainless steel	0.3 - 0.31
glass	0.18 - 0.3
concrete	0.1 - 0.2



3 situations

From Klawonn, Rheinbach et al 2008

$$\begin{aligned}\psi_A &= \psi^{\text{isochoric}} + \psi^{\text{volumetric}} + \psi^{\text{ti}} \\ &:= c_1 \left(\frac{I_1}{I_3^{1/3}} - 3 \right) + \epsilon_1 \left(I_3^{\epsilon_2} + \frac{1}{I_3^{\epsilon_2}} - 2 \right) + \sum_{i=1}^2 \alpha_1 \langle I_1 J_4^{(i)} - J_5^{(i)} - 2 \rangle^{\alpha_2}\end{aligned}$$

Set	Layer	c_1	ϵ_1	$\epsilon_2 (-)$	α_1	α_2	Purpose
D1	–	1.e3	1.e3	1.0	0.0	0.0	Deformations by different forces
C1	–	1.e3	1.e3	1.0	0.0	0.0	Different compressibility
C2	–	1.e3	1.e4	1.0	0.0	0.0	
C3	–	1.e3	1.e5	1.0	0.0	0.0	
A1	Adv.	7.5	100.0	20.0	1.5e10	20.0	Highly anisotropic arterial walls ¹
	Med.	17.5	100.0	50.0	5.0e5	7.0	
A2	Adv.	6.6	23.9	10	1503.0	6.3	
	Med.	17.5	499.8	2.4	30001.9	5.1	
A3	Adv.	7.8	70.0	8.5	1503.0	6.3	
	Med.	9.2	360.0	9.0	30001.9	5.1	

Table: Model parameter sets of ψ_A

¹kPa for $c_1, \epsilon_1, \alpha_1$.

Test for large deformation

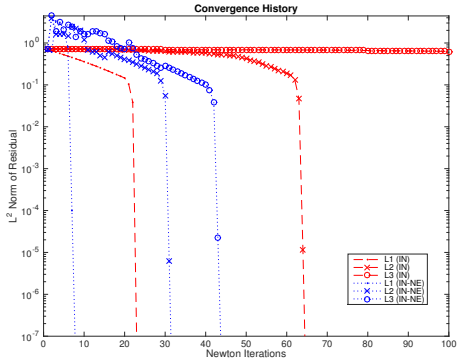


Figure: Convergence history of IN and IN-NE.

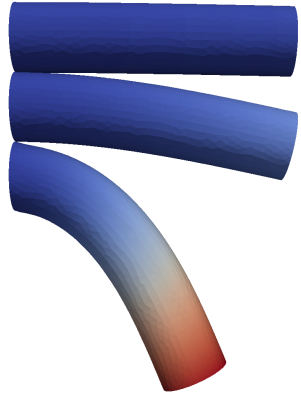


Figure: Deformations by different pulls.

Test for compressibility

For consistency with linear elasticity,

$$C_1 = \frac{\mu}{2}, \epsilon_1 = \frac{\kappa}{2},$$

where μ , κ and the shear and bulk modulus. The Poisson ratio can be computed by

$$\nu = \frac{3K - 2G}{2(3K + G)}$$

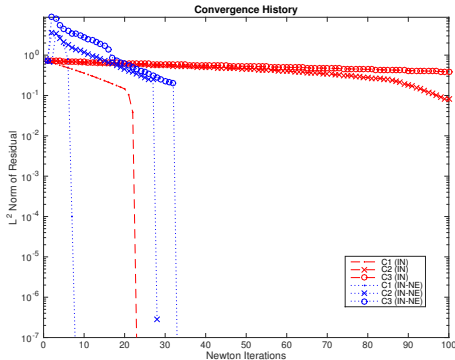


Figure: Convergence history of IN and IN-NE.

Set	Poisson's Ratio
C1	0.125
C2	0.452
C3	0.495

Test for anisotropic arterial wall

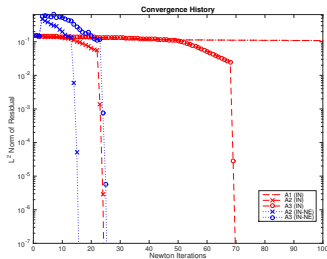


Figure: Convergence history of IN and IN-NE.

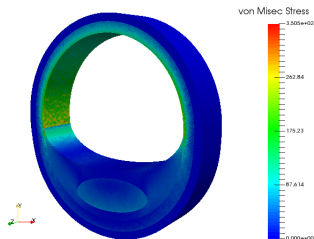


Figure: von Mises stress

Some final remarks

- For problems with uniform global nonlinearity, NKS is a good general purpose parallel solver. Multilevel maybe necessary if the number of processors is large
- For problems with unbalanced global and local nonlinearities, a combination of full space Newton and subspace Newton, in the form of a nonlinear elimination preconditioned Newton, offers a good strategy
- It may not be easy to identify the local 'bad' region
- For problems with only local nonlinearities, subspace Newton is often sufficient
- It is often difficult to tell what types of nonlinearities a problem may have
- The norm of the residual function, $\|F(x)\|_2$, is often not a good monitor, unfortunately all existing nonlinear theories and algorithms are based on $\|F(x)\|_2$
- Many parameters (stopping conditions)

Some recent publications

- L. Luo, X.-C. Cai, and D. Keyes, Nonlinear preconditioning strategies for two-phase flows in porous media discretized by a fully implicit discontinuous Galerkin method, SIAM J. Sci. Comput., (2021, to appear)
- L. Luo, X.-C. Cai, Z. Yan, L. Xu, and D. Keyes, A multi-layer nonlinear elimination preconditioned inexact Newton method for steady-state incompressible flow problems in 3D, SIAM J. Sci. Comput., 42 (2020), pp. B1404-1428
- L. Luo, W.-S. Shiu, R. Chen, and X.-C. Cai, A nonlinear elimination preconditioned inexact Newton method for blood flow problems in human artery with stenosis, J. Comp. Phys., 399 (2019), 108926
- S. Gong and X.-C. Cai, A nonlinear elimination preconditioned Newton method for heterogeneous hyperelasticity, SIAM J. Sci. Comput., 41 (2019), pp. S390-S408